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On computer simulation of Feynman–Kac path-integrals

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Abstract

Consider a path-integral $E_x \exp\{\int_0^t V(X(s))\,ds\} f(X(t))$ which is the solution to a diffusion version of the generalized Schrödinger's equation $\partial u/\partial t = Hu$, $u(0, x) = f(x)$. Here $H = A + V$, where A is an infinitesimal generator of a strongly continuous Markov semigroup corresponding to the diffusion process $\{X(s), 0 \leqslant s \leqslant t, X(0) = x\}$. To see a connection to quantum mechanics, take $A = \frac{1}{2}\Delta$ and replace V by $-V$. Then one obtains $\bar{H} = -H = -\frac{1}{2}\Delta + V$, which is a quantum mechanical Hamiltonian corresponding to a particle of mass 1 (in atomic units) subject to interaction with potential V. Path-integrals play a role in obtaining physical quantities such as ground state energies. This paper will be concerned with explanations of two approaches in the actual computer evaluations of path-integrals through simulations of the diffusion processes. The results will be presented by comparing, in concrete examples, the computational advantages or disadvantages depending on whether the diffusion process $X(t)$ is ergodic or not.

Keywords: Diffusion random walks; Harmonic oscillator; Hydrogen atom

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1. Introduction

A starting point of our analysis is the well-known Feynman–Kac representation of the solution to the initial value problem

$$\frac{\partial u(t, x)}{\partial t} = \tfrac{1}{2}\Delta u(t, x) - V(x)u(t, x), \quad t > 0, \; u(0, x) = 1, \tag{1.1}$$

given in the form of the path-integral with respect to the standard Brownian motion $X(t)$ with $X(0) = x$ as follows:

$$u(t, x) = E_x \exp\left\{-\int_0^t V(X(s))\,ds\right\}. \tag{1.2}$$

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It is known that the class of potentials V for which the above holds true is sufficiently large to accommodate singular potentials in quantum mechanics [6]. There are also some new results on the equivalence of Schrödinger and diffusion equations [5].

Our interest and motivation stems from numerical work done in [2–4] which served as a prototype for testing the feasibility of Eq. (1.2) while calculating the ground state energies of simple quantum systems.

It turns out that the representation (1.2) can be generalized [1] to employ a large class of diffusions that, unlike Brownian motion, have stationary distributions. More precisely, for any twice differentiable $\varphi(x) > 0$ define a new potential U which is a perturbation of the potential V as follows:

$$U(x) = V(x) - \frac{1}{2}\frac{\Delta\varphi(x)}{\varphi(x)}.$$

Furthermore, consider

$$v(t, x) = E_x \exp\left\{-\int_0^t U(Y(s))\,\mathrm{d}s\right\}, \tag{1.3}$$

which is the Feynman–Kac solution to

$$\frac{\partial v(t, x)}{\partial t} = \frac{1}{2}\Delta v(t, x) + \frac{\nabla\varphi(x)}{\varphi(x)}\cdot\nabla v(t, x) - U(x)v(t, x) \tag{1.4}$$

corresponding to the new diffusion $Y(t)$ with the infinitesimal generator

$$A = \frac{1}{2}\Delta + \frac{\nabla\varphi}{\varphi} \quad \text{with adjoint } A^*(\cdot) = \frac{1}{2}\Delta - \nabla\left(\frac{\nabla\varphi}{\varphi}(\cdot)\right). \tag{1.5}$$

Here $\varphi^2(x) > 0$ is a stationary probability density of $Y(t)$ or equivalently $A^*(\varphi^2) = 0$. To see now the connection between $v(t, x)$ in (1.3) and $u(t, x)$ in (1.2) observe that $v(t, x) = u(t, x)/\varphi(x)$ because $v(t, x)$ satisfies (1.4). See also Nagasawa's formula (3.68) in [5, p. 85] for generalizations.

We assume, in addition, that $\varphi(x) > 0$, i.e., no nodes are allowed and φ is square integrable. The only other stipulation, confirmed by numerical calculations, is that one should choose φ in the context of the available information about reasonable ground state trial functions (e.g., variational calculations for $-\frac{1}{2}\Delta + V$) and consider the Ito-type process $Y(t)$ which solves the following stochastic differential equation:

$$\mathrm{d}Y(t) = \frac{\nabla\varphi(Y(t))}{\varphi(Y(t))}\,\mathrm{d}t + \mathrm{d}X(t). \tag{1.6}$$

Sampling $Y(t)$ gives better rate of convergence to $v(t, x)$ than sampling $X(t)$ due to the drift component $(\nabla\varphi)/\varphi$ which forces the walk into the region where potential V affects quantum motion the most. Eventually one obtains the ground state energy λ_0 of H by taking the limit for large t as follows:

$$\lambda_0 = -\lim(1/t)\log v(t, x). \tag{1.7}$$

To ensure better convergence, $v(t, x)$ was sampled at various values $0 < t < 50$ and then the best nonlinear fit to $(1/t)\log v(t, x)$ on the semi-logarithmic scale using Levenberg–Marquardt method was applied. Various choices of φ correspond to a technique known as important sampling in the Monte Carlo literature.

2. Harmonic oscillator

In this section we will present calculations obtained for the one-dimensional harmonic oscillator with the Hamiltonian given by

$$-\frac{1}{2}\frac{d^2}{dx^2}+\frac{1}{2}x^2, \tag{2.1}$$

for which the ground state energy and the wave function are given, respectively, by $\lambda_0 = 0.5$ and $(1/\pi)^{1/4}\exp\{-\frac{1}{2}x^2\}$.

In all cases below, we have discretized the diffusion in both space and time by taking the random walk with $dx = \frac{1}{20}$ and $dt = (dx)^2$ to approximate (1.2), (1.3) and (1.6) while performing the actual computer simulations.

(a) *Regular Feynman–Kac formula*

$$\text{Npath} = 100\,000, \quad \bar{\lambda}_0 = 0.4966, \qquad \text{Npath} = 500\,000, \quad \bar{\lambda}_0 = 0.4983.$$

(b) *Important sampling (space average)*

We chose Cauchy-like distribution $\varphi(x) = \sqrt{(2/\pi)}\{1/(1+x^2)\}$ whose variational energy is $\frac{3}{4}$ (cf. $\lambda_0 = 0.5$),

$$\text{Npath} = 100\,000, \quad \bar{\lambda}_0 = 0.4987, \qquad \text{Npath} = 500\,000, \quad \bar{\lambda}_0 = 0.5003.$$

(c) *Important sampling (time average)*

Here instead of taking a large number of individual trajectories, Npath, we ran a single long trajectory and invoked the ergodicity of the process $Y(t)$ in evaluating the path-integral. Namely, the integral $I(t, T) = (1/T)\int_0^T \exp\{-\int_\tau^{\tau+t} U(Y(s))\,ds\}d\tau$ was appropriately discretized.

$$T = 1000, \qquad t = 10, \qquad \bar{\lambda}_0 = 0.4933,$$

$$T = 1000, \qquad t = 15, \qquad \bar{\lambda}_0 = 0.4957,$$

$$T = 10\,000, \qquad t = 20, \qquad \bar{\lambda}_0 = 0.5013.$$

3. Hydrogen atom

The most elaborate and demanding for computer time are bound state problems due to singularity of the potential. In our calculation for hydrogen atom with the Hamiltonian

$$-\frac{1}{2}\Delta - \frac{1}{\sqrt{x^2+y^2+z^2}}, \tag{3.1}$$

($\lambda_0 = -0.5$, ground state function $(1/\sqrt{\pi})\exp\{-(x^2+y^2+z^2)^{1/2}\}$), we have chosen gaussian $\varphi(x, y, z) = (1/\pi)^{3/4}\exp\{-\frac{1}{2}(x^2+y^2+z^2)\}$ for which the variational calculation gives the energy -0.3783 (cf. $\lambda_0 = -0.5$). The process $Y(t)$ is then the Ornstein–Uhlenbeck process with linear drift $(-x, -y, -z)$ toward the origin.

The results are as follows:

$$\text{Npath} = 500\,000, \quad \bar{\lambda}_0 = -0.50197, \qquad \text{Npath} = 1\,000\,000, \quad \bar{\lambda}_0 = -0.500041.$$

The nonlinear fit to the data taken from $t = 1$ step 1 to $t = 50$ utilized the first four differences between the bottom of the spectrum and the corresponding energies, i.e., $\lambda_i - \lambda_0$ with $\lambda_i = -1/2(i+1)^2$, $i = 0, 1, 2, 3, 4$. In other words, the fit was sought in the class of functions

$$a + \text{Log}[b + ce^{-0.375t} + de^{-0.4444t} + fe^{-0.4687t} + ge^{-0.48t}]/t,$$

where coefficients $a, \ldots, g$ were optimized and a served then as approximation to $\bar{\lambda}_0$.

To achieve a comparable result, i.e., three digits of accuracy, by using the standard Kac procedure (without the important sampling) it was found that the computing time must increase approximately eight-fold.

4. Conclusion

From these generic cases simulated on a serial computer (AXP-150 MHZ workstation by DEC, running a 64 bit alpha-chip) it is quite clear that without important sampling the original Feynman–Kac formula may not be numerically feasible. On the other hand, by combining the important sampling techniques with parallel computing (e.g., the Intel iPSC/860 with at least 32 processors or any other special purpose multiprocessor machines) one can satisfactorily treat quantum mechanical many-particle systems within a computing-time demand required by single particle calculations. This is possible due to parallel computer architecture which allows for independent and simultaneous computations corresponding to each particle in the system. Calculations for many-particle systems, including fermions and excited states with their corresponding nodal surfaces, are currently under way and will be submitted elsewhere.

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